

10092889

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* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 JAN 27 Source of Registration (SR) information in REGISTRY updated
and searchable
NEWS 4 JAN 27 A new search aid, the Company Name Thesaurus, available in
CA/CAPLUS
NEWS 5 FEB 05 German (DE) application and patent publication number format
changes
NEWS 6 MAR 03 MEDLINE and LMedline reloaded
NEWS 7 MAR 03 MEDLINE file segment of TOXCENTER reloaded
NEWS 8 MAR 03 FRANCEPAT now available on STN
NEWS 9 MAR 29 Pharmaceutical Substances (PS) now available on STN
NEWS 10 MAR 29 WPIFV now available on STN
NEWS 11 MAR 29 No connect hour charges in WPIFV until May 1, 2004
NEWS 12 MAR 29 New monthly current-awareness alert (SDI) frequency in RAPRA
NEWS 13 APR 26 PROMT: New display field available
NEWS 14 APR 26 IFIPAT/IFIUDB/IFICDB: New super search and display field
available
NEWS 15 APR 26 LITAlert now available on STN
NEWS 16 APR 27 NLDB: New search and display fields available

NEWS EXPRESS MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
NEWS HOURS STN Operating Hours Plus Help Desk Availability
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NEWS PHONE Direct Dial and Telecommunication Network Access to STN
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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 10:29:05 ON 10 MAY 2004

10092889

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

ENTRY

TOTAL

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 10:29:17 ON 10 MAY 2004

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STRUCTURE FILE UPDATES: 9 MAY 2004 HIGHEST RN 680971-82-8

DICTIONARY FILE UPDATES: 9 MAY 2004 HIGHEST RN 680971-82-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10092889e.str

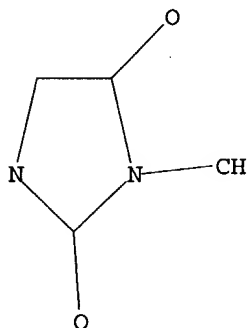
L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

CF₃



Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam

SAMPLE SEARCH INITIATED 10:29:34 FILE 'REGISTRY'

10092889

SAMPLE SCREEN SEARCH COMPLETED - 112 TO ITERATE

100.0% PROCESSED 112 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1606 TO 2874
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 10:29:38 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2078 TO ITERATE

100.0% PROCESSED 2078 ITERATIONS 20 ANSWERS
SEARCH TIME: 00.00.01

L3 20 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS
FULL ESTIMATED COST

	SINCE FILE ENTRY	TOTAL SESSION
	155.42	155.63

FILE 'CAPLUS' ENTERED AT 10:29:42 ON 10 MAY 2004
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FILE COVERS 1907 - 10 May 2004 VOL 140 ISS 20
FILE LAST UPDATED: 9 May 2004 (20040509/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L4 2 L3

=> d l4 1-2 ibib abs hitstr

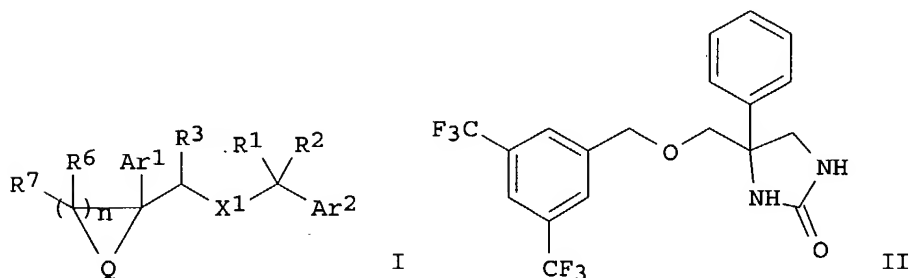
L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:453028 CAPLUS
DOCUMENT NUMBER: 135:61331
TITLE: Preparation of 2-imidazolidinones and related compounds as selective neurokinin antagonists

10092889

INVENTOR(S): Shih, Neng-Yang; Shue, Ho-Jane; Reichard, Gregory A.;
Paliwal, Sunil; Blythin, David J.; Piwinski, John J.;
Xiao, Dong; Chen, Xiao
PATENT ASSIGNEE(S): Schering Cooperation, USA
SOURCE: PCT Int. Appl., 108 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001044200	A2	20010621	WO 2000-US33831	20001214
WO 2001044200	A3	20011213		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PL, PT, RO, RU, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6436928	B1	20020820	US 2000-737036	20001214
US 2002123491	A1	20020905		
EP 1237874	A2	20020911	EP 2000-984340	20001214
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003522739	T2	20030729	JP 2001-544690	20001214
US 2003064980	A1	20030403	US 2002-163663	20020606
US 6635630	B2	20031021		
PRIORITY APPLN. INFO.:				
			US 1999-172489P	P 19991217
			US 2000-737036	A3 20001214
			WO 2000-US33831	W 20001214

OTHER SOURCE(S): MARPAT 135:61331
GI



AB Title compds. [I; wherein Ar1 and Ar2 = (un)substituted heteroaryl or Ph; X1 = O, S, SO, SO2, NR12, NCOR12, or NR12SO2R15; Q = X2C(:Y)N(R4), N:C(Y1)N(R4), X2C(Y1):N, or N(R5)SO2N(R4); X2 = O, S, or NR5; Y = O, S, or NR11; Y1 = H, alkyl, SMe, alkoxy-carbonylaminoalkyl, NHCOR15, or (un)substituted amino, urea, (hetero)aryl(alkyl), or heterocycloalkyl; n =

1-4; R1, R2, R3 and R7 = H, (cyclo)alkyl, CHF2, CH2F, or CF3; or R1 and R2 together with the C to which they are attached form an alkylene ring; or R1 and R2 together are :O; R4 and R12 = independently H or (cyclo)alkyl; R5 = H or (CH2)mG; m = 0-5; G = H, CF3, CHF2, CH2F, (cyclo)alkyl, (hetero)aryl, OH, (cyclo)alkoxy, SO2R13, (un)substituted amino, sulfamoyl, sulfonylamino, acylamino, carbamoyl, carboxy, urea, etc. with provisos; R6 = R7 or OH with provisos; R11 = H, (cyclo)alkyl, NO2, CN, OH, alkoxy, carbamoyl(alkyl), (hetero)aryl(alkyl), etc.; R13 = H, (cyclo)alkyl, or (hetero)aryl(alkyl), etc.; R15 = (cyclo)alkyl or CF3] were prepared as selective neurokinin antagonists. For example, cycloaddn. of (NH4)2CO3 to 2-[[3,5-bis(trifluoromethyl)phenyl]methoxy]-4'-fluoroacetophenone (4-step preparation given) afforded the 2,4-imidazolidinedione (82%), which was reduced with LAH-AlCl3 (82%). Resolution of the racemates on a chiral column, followed by recrystn., gave the imidazolidinone (-)-II. I exhibited a range of NK1 antagonist activity with Ki values ranging from about 0.1 nM to 1000 nM. Thus, I and pharmaceutical compns. of I in combination with selective serotonin reuptake inhibitors are useful in the treatment of emesis, depression, anxiety, cough, and other NK1-related disorders (no data).

IT 345579-87-5P 345580-00-9P 345580-07-6P

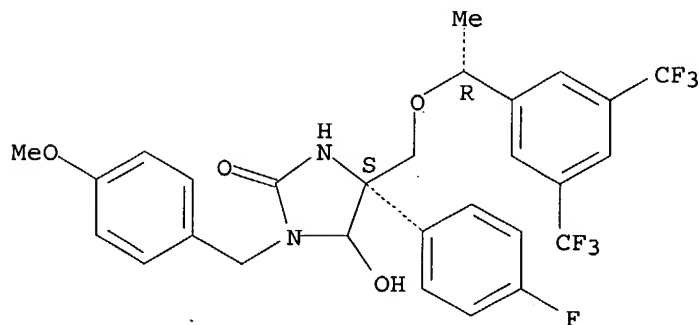
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of 2-imidazolidinones and related compds. as selective neurokinin antagonists via cycloaddn. reactions)

RN 345579-87-5 CAPLUS

CN 2-Imidazolidinone, 4-[[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-4-(4-fluorophenyl)-5-hydroxy-1-[(4-methoxyphenyl)methyl]-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

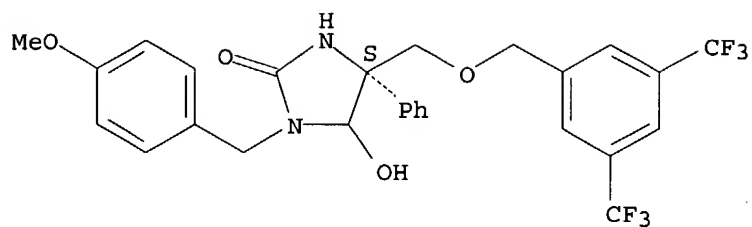


RN 345580-00-9 CAPLUS

CN 2-Imidazolidinone, 4-[[[3,5-bis(trifluoromethyl)phenyl]methoxy]methyl]-5-hydroxy-1-[(4-methoxyphenyl)methyl]-4-phenyl-, (4S)- (9CI) (CA INDEX NAME)

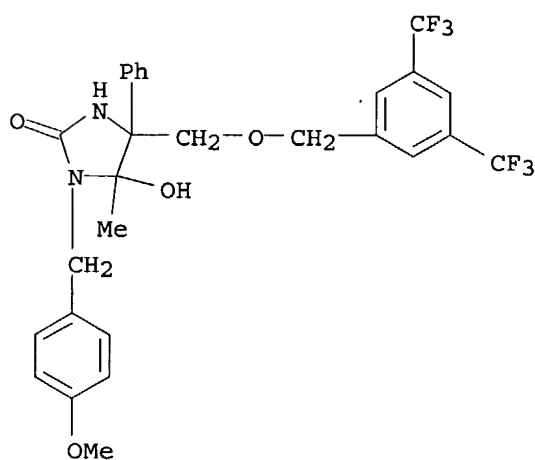
Absolute stereochemistry.

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RN 345580-07-6 CAPLUS

CN 2-Imidazolidinone, 4-[[[3,5-bis(trifluoromethyl)phenyl]methoxy]methyl]-5-hydroxy-1-[(4-methoxyphenyl)methyl]-5-methyl-4-phenyl- (9CI) (CA INDEX NAME)



IT 345580-27-0P 345580-28-1P

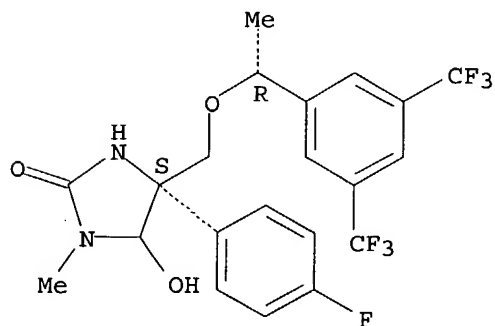
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(preparation of 2-imidazolidinones and related compds. as selective neurokinin antagonists via cycloaddn. reactions)

RN 345580-27-0 CAPLUS

CN 2-Imidazolidinone, 4-[[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-4-(4-fluorophenyl)-5-hydroxy-1-methyl-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

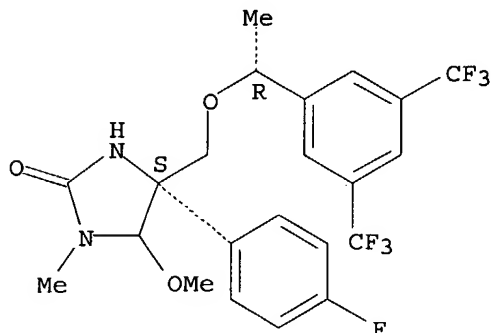


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RN 345580-28-1 CAPLUS

CN 2-Imidazolidinone, 4-[[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-4-(4-fluorophenyl)-5-methoxy-1-methyl-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 345578-85-0P 345578-86-1P

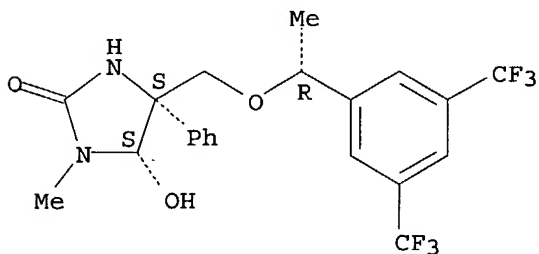
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PUR (Purification or recovery); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of 2-imidazolidinones and related compds. as selective neurokinin antagonists via cycloaddn. reactions)

RN 345578-85-0 CAPLUS

CN 2-Imidazolidinone, 4-[[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-5-hydroxy-1-methyl-4-phenyl-, (4S,5S)- (9CI) (CA INDEX NAME)

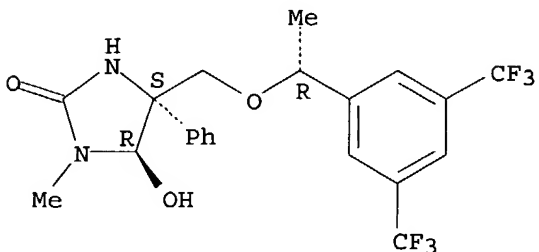
Absolute stereochemistry.



RN 345578-86-1 CAPLUS

CN 2-Imidazolidinone, 4-[[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-5-hydroxy-1-methyl-4-phenyl-, (4S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



10092889

IT 345578-91-8P 345578-92-9P 345579-13-7P
345579-14-8P

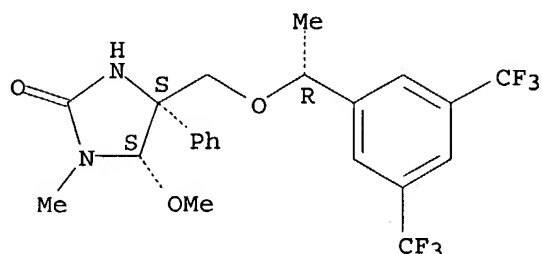
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 2-imidazolidinones and related compds. as selective neurokinin antagonists via cycloaddn. reactions)

RN 345578-91-8 CAPLUS

CN 2-Imidazolidinone, 4-[[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-5-methoxy-1-methyl-4-phenyl-, (4S,5S)- (9CI) (CA INDEX NAME)

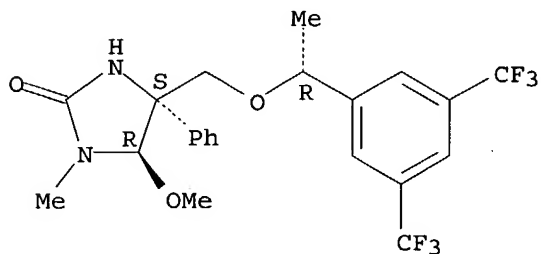
Absolute stereochemistry.



RN 345578-92-9 CAPLUS

CN 2-Imidazolidinone, 4-[[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-5-methoxy-1-methyl-4-phenyl-, (4S,5R)- (9CI) (CA INDEX NAME)

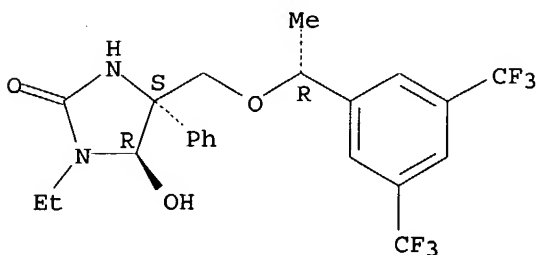
Absolute stereochemistry.



RN 345579-13-7 CAPLUS

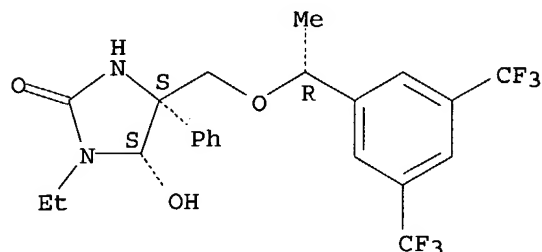
CN 2-Imidazolidinone, 4-[[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-1-ethyl-5-hydroxy-4-phenyl-, (4S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



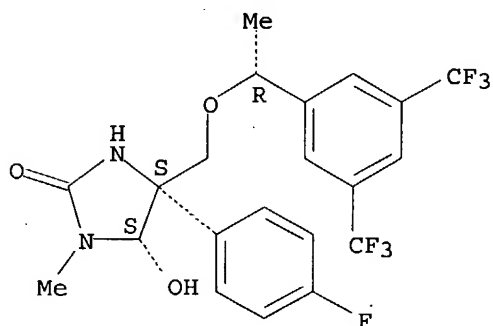
RN 345579-14-8 CAPLUS

Absolute stereochemistry.



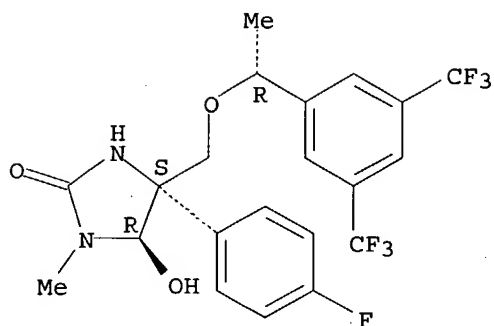
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-imidazolidinones and related compds. as selective neurokinin antagonists via cycloaddn. reactions)

Absolute stereochemistry.



Absolute stereochemistry.

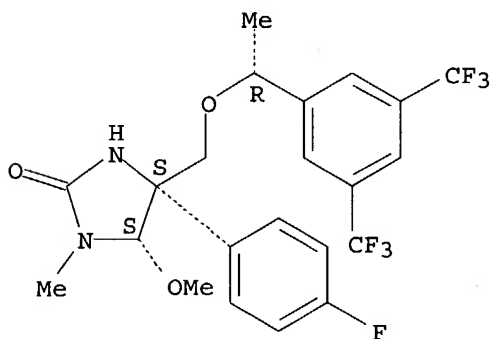
10092889



RN 345578-70-3 CAPLUS

CN 2-Imidazolidinone, 4-[[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-4-(4-fluorophenyl)-5-methoxy-1-methyl-, (4S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 345578-11-2P 345578-14-5P

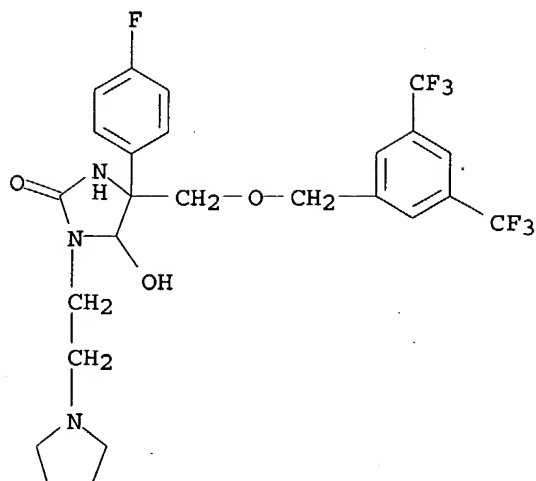
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of 2-imidazolidinones and related compds. as selective neurokinin antagonists via cycloaddn. reactions)

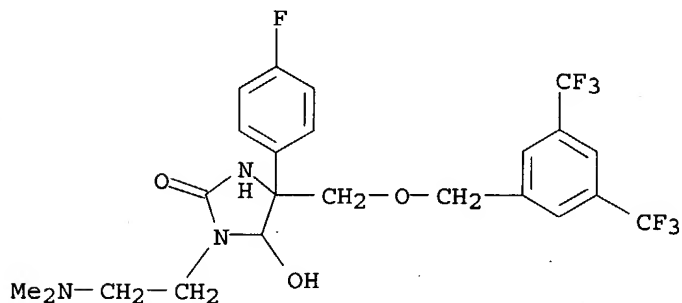
RN 345578-11-2 CAPLUS

CN 2-Imidazolidinone, 4-[[[3,5-bis(trifluoromethyl)phenyl]methoxy]methyl]-4-(4-fluorophenyl)-5-hydroxy-1-[2-(1-pyrrolidinyl)ethyl]- (9CI) (CA INDEX NAME)

10092889

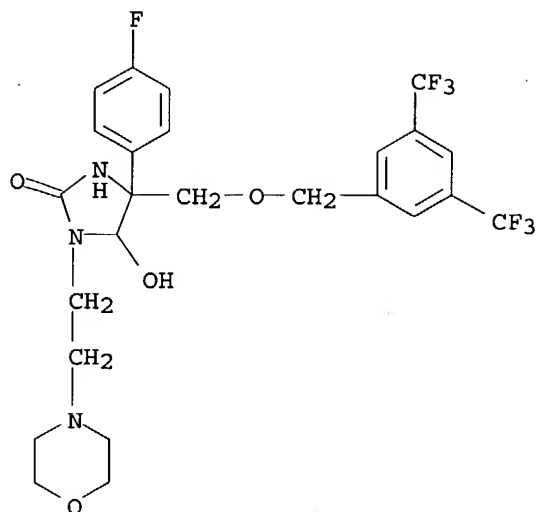


RN 345578-14-5 CAPLUS
CN 2-Imidazolidinone, 4-[[[3,5-bis(trifluoromethyl)phenyl]methoxy]methyl]-1-[2-(dimethylamino)ethyl]-4-(4-fluorophenyl)-5-hydroxy- (9CI) (CA INDEX NAME)



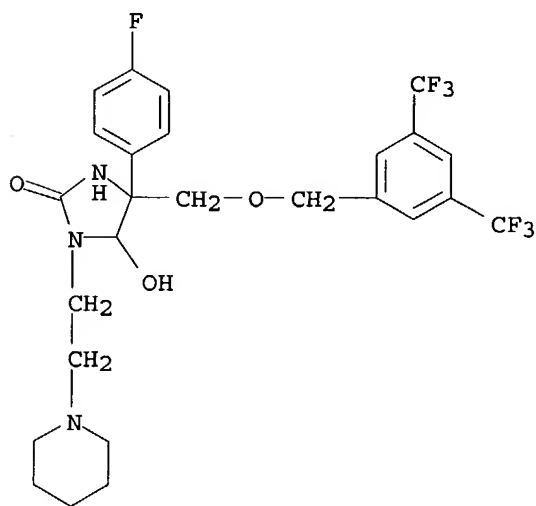
IT 345578-01-0P 345578-03-2P 345580-26-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-imidazolidinones and related compds. as selective neurokinin antagonists via cycloaddn. reactions)
RN 345578-01-0 CAPLUS
CN 2-Imidazolidinone, 4-[[[3,5-bis(trifluoromethyl)phenyl]methoxy]methyl]-4-(4-fluorophenyl)-5-hydroxy-1-[2-(4-morpholinyl)ethyl]- (9CI) (CA INDEX NAME)

10092889



RN 345578-03-2 CAPLUS

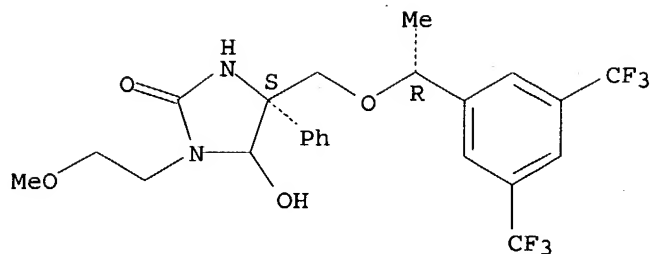
CN 2-Imidazolidinone, 4-[[[3,5-bis(trifluoromethyl)phenyl]methoxy]methyl]-4-(4-fluorophenyl)-5-hydroxy-1-[2-(1-piperidiny)ethyl]- (9CI) (CA INDEX NAME)



RN 345580-26-9 CAPLUS

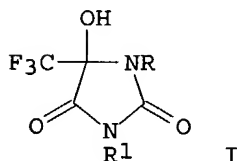
CN 2-Imidazolidinone, 4-[[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-5-hydroxy-1-(2-methoxyethyl)-4-phenyl-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1987:50220 CAPLUS
 DOCUMENT NUMBER: 106:50220
 TITLE: 5-Hydroxy-5-(trifluoromethyl)-2,4-imidazolidinediones
 INVENTOR(S): Takaoka, Akio; Ishikawa, Nobuo; Iwa, Riichi
 PATENT ASSIGNEE(S): Nippon Mectron Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61197561	A2	19860901	JP 1985-35364	19850226
JP 05048226	B4	19930720		
PRIORITY APPLN. INFO.: GI			JP 1985-35364	19850226



AB The title compds. (I; R, R1 = H, alkyl), potentially useful as virucides, neoplasm inhibitors, and herbicides, or as intermediates therefor, were prepared by reaction of trifluoropyruvic acid hydrate (II) with urea, or mono- or dialkylureas. Thus, refluxing II (prepared by autoclaving hexafluoropropylene oxide with H2O, Et2O, and silica gel) and urea in EtOH for 24 h gave 61% I (R = R1 = H).

IT **106289-13-8P**, 5-Hydroxy-5-trifluoromethyl-1-methylimidazolidine-2,4-dione
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 106289-13-8 CAPLUS

CN 2,4-Imidazolidinedione, 5-hydroxy-1-methyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

10092889

